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VALIDATION OF CONTAMW PREDICTIONS FOR TRACER GAS IN A TOWNHOUSE

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ABSTRACT

To provide additional validation data for the multizone airflow and contaminant model, CONTAMW, experiments were performed in an occupied 3-story townhouse in Reston, VA. A tracer gas, sulfur hexaflouride (SF_6), was manually injected within one room of the house and the concentration of SF_6 was measured in each zone. This same process was then recreated in CONTAMW and the resulting predictions were statistically compared to the measured values. A total of 10 experiments were conducted and simulated between May 2000 and June 2001. The tests involved injecting 1500 mL of 1 % SF_6 in a single room of the house. In 4 of the 10 cases, the heating and air-conditioning system fan was operating. SF_6 was injected in the Recreation Room (basement level), the Kitchen/Dining Room (main level) and the Master Bedroom (upstairs level). Ambient conditions ranged from a low outdoor temperature of 5 °C to a high of 29 °C. Wind conditions ranged from calm to moderate with a high average wind speed of 4 m/s.

A statistical comparison of measurements and predictions was performed per ASTM D5157 (ASTM 1997) for all cases. Comparisons were made for overall zone average concentrations and individual zone transient concentrations. The results for zone average concentrations were very good with many cases meeting most or all of the D5157 criteria. Several cases showed a poor to fair correlation between average measurements and predictions due to discrepancies with a single zone - the main floor bathroom - but excluding that zone resulted in these cases meeting or nearly meeting the D5157 criteria. Comparisons of individual zone transient concentrations were mixed with many good to excellent cases but also numerous fair to poor. As expected, there were frequently large differences between measured and predicted peak concentrations. Also, the bathroom zone was a consistently difficult zone to predict accurately. Other zones had occasional poor comparisons between predictions and measurements but no consistent discrepancies. The predicted SF_6 concentration averaged over all zones and cases was within 10 % of the average measured concentration. Excluding the bathroom zone, the overall average predicted concentration (115 µg/m^3) was essentially identical to the overall average measured concentration (116 µg/m^3).

INTRODUCTION

There are two general types of computer simulation techniques for studying airflow and contaminant transport in buildings – zonal modeling and multizone modeling. Zonal (or room airflow) modeling takes a microscopic view by applying a computational fluid dynamics (CFD) program to examine the detailed flow fields and pollutant concentration distributions within a room or rooms. Multizone airflow and pollutant transport modeling takes a macroscopic view by evaluating average pollutant concentrations in the different zones of a building as contaminants are transported through the building and its heating and air-conditioning (HAC) system. Each approach has strengths and limitations for studying different aspects of building ventilation and indoor air quality (IAQ).

The multizone approach is implemented by constructing a network of elements, describing the flow paths (HAC ducts, doors, windows, cracks, etc.) between the zones of a building. The network nodes represent the zones, which are modeled at a uniform pressure, temperature, and pollutant concentration. After calculating the airflow between zones, including the outdoors, zonal pollutant concentrations are calculated by applying mass balance equations to the zones, which may contain pollutant sources and/or sinks. Feustel and Dieris (1992) described a survey of multizone airflow models. One multizone model is the CONTAM model developed in the Building and Fire Research Laboratory (BFRL) at the National Institute of Standards and Technology (NIST). The newest publicly available version of CONTAM is CONTAMW 2.0 (Dols et al. 2002).

Multizone indoor air quality (IAQ) modeling has been available as a research and analysis tool for over 20 years. However, due to improvements in such modeling programs (e.g., graphical user interfaces), the application of such programs has greatly increased and is moving from the research world to a broader audience. This has, in turn, increased the need for establishing the validity of these models.

This paper describes experiments and simulations performed to evaluate the capability to accurately simulate tracer gas concentrations with a multizone airflow and IAQ model, in this case CONTAMW. Measurements of tracer gas concentrations were performed in a multizone townhouse. Additional detail on the experiments and simulations may be found in a separate report (Emmerich et al. 2003).

EXPERIMENTAL PROCEDURE

Test House

The test house is a three-story end-unit townhouse with an approximate floor area of 50 m^2 per level and an approximate overall volume of 400 m^3. The townhouse is located 35 km NW of Washington, D.C. The townhouse has a partial basement consisting of a pantry, utility room, bathroom, and recreation room with walkout patio. The middle level consists of a kitchen, dining room, living room, and bathroom. The top level contains four bedrooms and two bathrooms (Figure 1). The townhouse's heating and air-conditioning (HAC) system uses 100% recirculated air and its ductwork does not enter the attic, resulting in no direct duct leakage to or from outside. Two blower door tests (ASTM E779) were performed (May 1999 and July 2000) to assess the envelope leakage of the house. The closed house air change rate at 50 Pa averaged 14.2 h^{-1} with an effective leakage area of 1121 cm^2 at 4 Pa.

Instrumentation

Tracer gas, sulfur hexafluoride (SF_6), concentrations were measured using an automated tracer gas measurement system consisting of a PC-based data acquisition and control system and a gas chromatograph (GC) with an electron capture detector (ECD). The GC-ECD was used to determine SF_6 concentrations over a range of about 30 μg/m^3 to 900 μg/m^3 (5 ppb(v) to 150 ppb(v)) with an accuracy of approximately 2 %. The tracer gas system uses a ten-port sample valve to sample air at ten indoor locations every 10 minutes. The sample locations included the utility and recreation rooms on the basement level, kitchen, bathroom, and living rooms on the main level, master bedroom and two offices on the upstairs level, the attic, and the central return of the HAC system as seen on the test house floorplan shown in Figure 1. Most single point sample probes were located near the wall and many near the floor. Early measurements found no SF_6 in the outdoor air; the outdoor concentration of SF_6 was assumed to be zero for the remainder of the effort.

Indoor and outdoor temperatures were measured with thermistors having an uncertainty of about 0.4 °C. Wind speed and direction were measured using a sonic anemometer installed on the townhouse roof about 2 m above the crest of the roof.

A hot wire anemometer (HWA) with an uncertainty of 2.5 % was mounted at a point representative of the average velocity in the return duct to monitor duct airflow velocity during the tests. The average measured supply flow was 530 L/s and the average

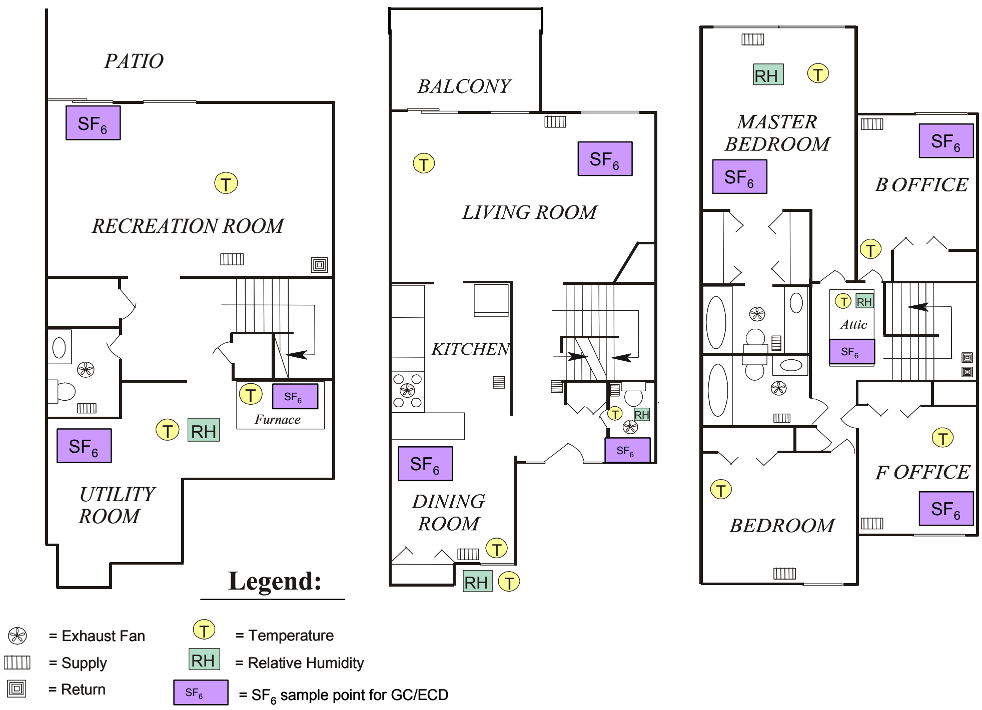

Figure 1 Schematic Floorplan of Townhouse

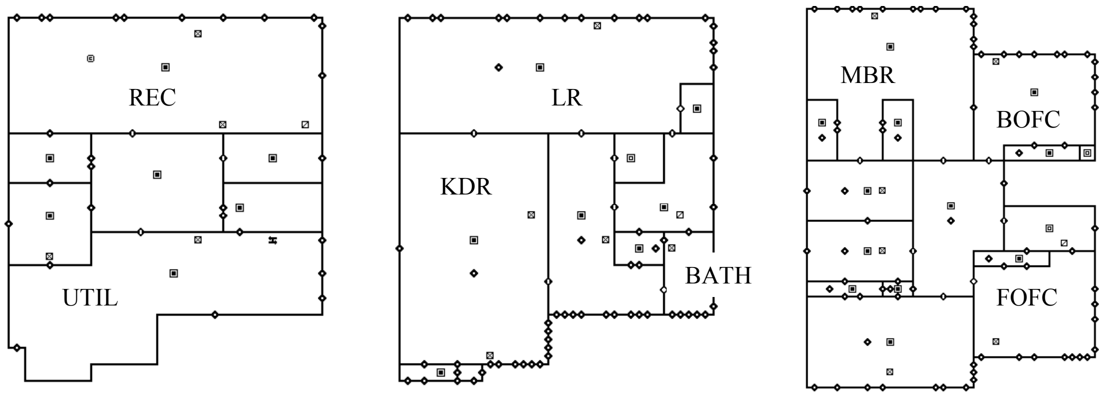

Figure 2 CONTAMW Sketchpad of Townhouse

measured return flow was 675 L/s. While the HAC system was operating, a balometer with an estimated accuracy of 10 % was used to measure the individual HAC system supply flows. After accounting for flows that were not measurable, the sum of measured supplies agreed reasonably well with the results of the traverse test. The CONTAMW simple air handling system (AHS) model was used to implement supply airflows based on the balometer measurements in the model. Attempts were made to measure the system return flows with the balometer also, however, accurate measurements were not possible due to the locations and magnitudes of those flows. Therefore, the total modeled system supply flow of 580 L/s was distributed equally between the 3 system returns shown in Figure 1. Since a system duct leakage test confirmed the presence of significant leakage, a 19 L/s supply duct leak located in the utility room was also included in the model.

SIMULATION PROCEDURE

The graphical representation of the three main floors of the test house as it appears in CONTAMW is shown in Figure 2. The townhouse attic was included in the model as a single zone but is not shown. The layout of the townhouse within CONTAMW and the division of the zones (including those not labeled) were set to represent the actual floorplan of the townhouse as seen in Figure 1. The zones labeled in Figure 2 correspond to the zones in which the injections took place and locations of measured concentrations.

Individual air leakage elements were created in CONTAMW based on best estimate values from Table 26-1 of the ASHRAE Handbook of Fundamentals (ASHRAE 2001). Then, the total leakage was adjusted such that the resulting flows from a simulated blower door test matched those from the real blower door test mentioned earlier.

To account for the effect of wind on a building, CONTAMW requires user inputs for a wind pressure modifier to account for local terrain effects and a wind pressure profile to account for relative wind direction (see Dols et al. 2000 for details on modeling wind effects in CONTAMW). Since the townhouse is almost surrounded by tall trees, the CONTAMW default wind pressure modifiers for an urban location were used. This decision was supported by the observation that wind has a minimal impact on infiltration in the house (Wallace 2002). The wind pressure profile was based on Figure 16.6 of the ASHRAE Handbook of Fundamentals (ASHRAE 2001).

A sample CONTAMW project file with all leakage elements, air handling system flows, and wind pressure data is available on the NIST Multizone Modeling Website at www.bfrl.nist.gov/IAQanalysis.

RESULTS

Statistical Evaluation of Model Predictions

The tracer gas predictions were compared with measured values using ASTM D5157 Standard Guide for Statistical Evaluation of Indoor Air Quality Models. This standard presents quantitative and qualitative tools for evaluation of IAQ models (ASTM 1997). It provides guidance in choosing data sets for model evaluation and focuses on evaluating the accuracy of indoor concentrations predicted by a model. The data sets collected during this study meet the ASTM D5157 criteria for model evaluation, as they are entirely independent of the data used to develop the model and to estimate model inputs. Also, the data are of sufficient temporal and spatial detail to evaluate the CONTAMW predictions of individual zonal tracer gas concentrations.

ASTM D5157 provides three statistical tools for evaluating the accuracy of IAQ model predictions and two additional statistical tools for assessing bias. Values for these statistical criteria are provided to indicate whether the model performance is adequate.

The tools for assessing agreement between predictions and measurements include:

1) The correlation coefficient of predictions and measurements should be 0.9 or greater.

2) The line of regression between the predictions and measurements should have a slope between 0.75 and 1.25 and an intercept less than 25 % of the average measured concentration.

3) The normalized mean square error (NMSE) should be less than 0.25. The NMSE is calculated as:

$$NMSE = \sum_{i=1}^{N} (C_{pi} - C_{oi})^2 \, / \, 2\overline{C}_o \overline{C}_p \quad (8)$$

where C_p is the predicted concentration and C_o is the observed concentration, and the over-bar represents an average over the N data points during the test period for each test case.

ASTM D5157 also provides two statistical measures of bias with values for judging adequate model performance. These measures of bias include:

1) Normalized fractional bias (FB) of the mean concentrations. Fractional bias should be 0.25 or lower and is calculated as:

$$FB = 2(\overline{C}_p - \overline{C}_o) / \left(\overline{C}_p + \overline{C}_o\right) \quad (9)$$

2) Fractional bias based on the variance (FS) which should be 0.5 or lower. FS is calculated as:

$$FS = 2(\sigma_p{}^2 - \sigma_o{}^2) / \left(\sigma_p{}^2 + \sigma_o{}^2\right) \quad (10)$$

where σ_p is the standard deviation of the predicted concentrations and σ_o is the standard deviation of the observed concentrations.

Comparison of Tracer Gas Predictions and Measurements

A total of ten experiments were conducted and simulations performed under a variety of conditions during tests conducted between May 2000 and June 2001. The tests consisted of injecting 1500 mL of tracer gas (1% SF_6) and measuring the concentration for two to six hours. The suggested ASTM D5157 statistical criteria were evaluated for both individual zone transient concentrations and overall zone average concentrations for the entire testing period for all cases. Two of the ten cases are shown and discussed below, one with the HAC fan on and one without.

Case # 2

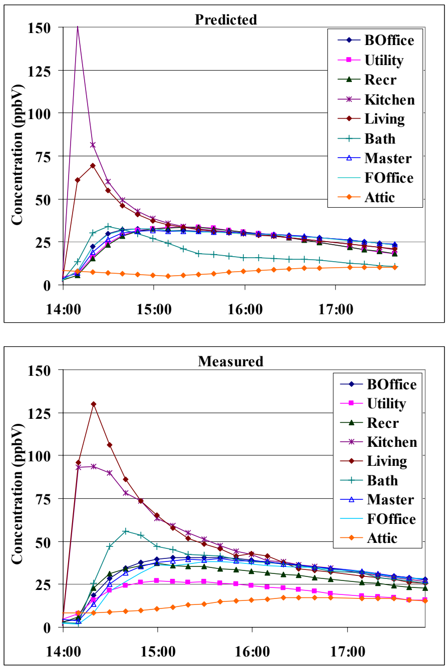

Figure 3 Predicted and Measured Concentrations for Case #2

Case #2 involved an injection in the KDR zone with the HAC system off. The average outdoor temperature was warm at 24.4 °C and the average wind speed was 1.3 m/s. The measured and predicted SF_6 concentrations for the individual zones are shown in Figure 3.

Table 1 presents the average observed concentration (C_o), average predicted concentration (C_p), standard deviation of observed concentrations (σ_o), standard deviation of predicted concentrations (σ_p), correlation coefficient (R), regression slope (m), regression intercept divided by the average observed concentration (b/C_o), normalized mean square error (NMSE), fractional bias of the mean concentrations (FB), and fractional bias based on the variance (FS) for the individual zone transient concentrations – recreation room (REC), utility room (UTIL), living room (LR), kitchen/dining room (KDR), master bedroom (MBR), back office (BOFC), front office (FOFC), main floor bathroom (BATH), and attic (ATC). The last row of the table presents the average of the nine zone concentrations (not weighted by zone size) and the statistical parameters for the time-averaged zone concentrations. The bold values in the table are those that met the D5157 suggested criteria.

Based on statistical parameters, this case resulted in fair overall agreement between measured and predicted values. Specifically, the values for R, m, and FS calculated for the comparison of average zone concentrations all fall outside the ASTM D5157 suggested limits. However, much of the discrepancy is due to a single zone, BATH, which was a

Table 1 Statistical Parameters for Case # 2

Zone	C_o	C_p	σ_o	σ_p	R	m	b/C_o (%)	NMSE	FB	FS
REC	28.2	24.7	8.8	8.7	**0.97**	**0.95**	**-7.7**	**0.02**	**-0.13**	**-0.03**
UTIL	20.6	25.0	5.9	8.4	**0.99**	1.4	**-19**	**0.05**	**0.19**	0.66
LR	50.6	32.6	30	14	**0.98**	0.47	**17**	0.33	**-0.43**	-1.2
KDR (inj. zone)	48.7	37.6	24	29	0.81	**0.98**	**-21**	**0.21**	**-0.26**	**0.39**
MBR	31.2	26.1	10	7.3	**0.96**	0.67	**17**	**0.05**	**-0.17**	-0.69
BOFC	32.1	26.5	10	7.4	**0.95**	0.67	**15**	**0.05**	**-0.19**	-0.67
FOFC	29.4	26.4	11	7.4	0.85	0.58	32	**0.05**	**-0.11**	-0.73
BATH	34.8	18.0	13	7.8	0.73	0.43	**8.2**	0.56	**-0.64**	-0.96
ATC	13.9	8.0	3.4	1.8	0.64	0.34	**24**	0.34	**-0.52**	-1.1
Average Concentrations	*32.2*	*25.0*	*12*	*8.4*	*0.81*	*0.57*	***20***	***0.12***	***-0.25***	*-0.67*

particularly difficult zone to model for test cases with the HAC fan off. Excluding the BATH zone from consideration increases R to 0.9 for the average concentrations and also brings all the other statistical parameters very close to the ASTM suggested limits. On average, the model under-predicts the zone average concentrations by about 20 % and, as Figure 3 shows, predicts mixing throughout the house to occur more quickly than measured.

One possible explanation for the under-prediction in he BATH zone is too much air leakage in the model with predicted infiltration in this zone much higher than any other zone. Although the BATH zone has the most wall area relative to the zone volume and therefore higher infiltration may be expected, the difference seems larger than it should be. However, no measurements were made to characterize the leakiness of individual zones. Also, the airflow element connecting the BATH zone to the adjacent hallway in the model is a two-way airflow element that estimates mixing between the zones based on the temperature difference between the zones. For this case, the average temperature difference between the indoor and outdoor is only 0.2 °C and between zones is only 0.3 °C.

Despite the injection occurring in the KDR zone, the measured peak concentration in the LR zone was higher. This result is not too surprising as the measurement locations for the two zones (near the east wall of the LR and the west wall of the KDR) were nearly the same distance from the injection location in the middle of the kitchen space of the KDR zone.

Case #7

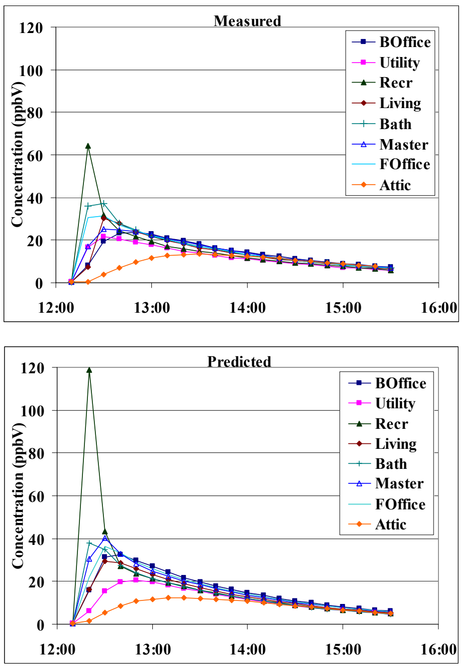

Figure 4 Predicted and Measured Concentrations for Case #7

Case #7 involved an injection in the REC zone with the HAC system operating during cold ambient conditions (6.7 °C). The measured and predicted transient zone concentrations are shown in Figure 4 and the D5157 statistical parameters are presented in Table 2. In this case, and in others, when the HAC system was on, the KDR zone was excluded from statistical analysis because the measuring point in this zone was located directly above the supply vent. With the system on, the measured values were not indicative of zone concentrations and therefore were

Table 2 Statistical Parameters for Case #7

Zone	C_o	C_p	σ_o	σ_p	R	m	b/C_o (%)	NMSE	FB	FS
REC (inj. zone)	15.3	18.9	13	25	**0.98**	1.8	**-60**	0.52	**0.21**	1.1
UTIL	11.8	11.2	5.5	5.8	0.87	**0.91**	**4.3**	**0.06**	**-0.05**	**0.09**
LR	13.8	14.1	7.6	8.0	**0.96**	**1.0**	0	**0.02**	**0.02**	**0.12**
KDR	12.1	14.3	*	*	*	*	*	*	*	*
MBR	14.5	16.3	6.7	10	**0.94**	1.4	**-32**	**0.10**	**0.12**	0.82
BOFC	13.9	16.0	6.3	9.0	**0.94**	1.4	**-20**	**0.08**	**0.14**	0.69
FOFC	15.2	16.0	8.3	9.6	**0.96**	**1.1**	**-4.8**	**0.04**	**0.05**	**0.28**
BATH	15.7	14.4	9.5	10	**0.99**	**1.0**	**-12**	**0.01**	**-0.08**	**0.09**
ATC	9.34	8.34	3.9	3.5	**0.94**	**0.83**	**5.9**	**0.04**	**-0.11**	**-0.23**
Average Concentrations	*13.5*	*14.5*	*2.1*	*3.1*	*0.86*	***1.3***	***-21***	***0.02***	***0.06***	*0.74*

excluded. As expected with HAC system on, there was very good agreement between predictions and measurements for both individual zone transient concentrations and zone average concentrations. Just a few parameters fell outside the D5157 criteria and mostly not by much. In addition the predicted and measured concentrations in the HAC central return agreed very well with a correlation coefficient of 1.0 and overall average predicted concentration exceeding measured by less than 10 %.

There is a large difference between measured and predicted peak concentrations for this case and most others. There are several reasons for this. First, since there was no attempt to mix the tracer gas once injected into a zone, peak values measured may not be representative of the entire zone. Also, neither experiments nor simulations were specifically designed to account for short-term peaks. Effort was made to match the timing of the predicted peak concentrations to measured values, but only within about ten minutes.

DISCUSSION

Table 4 summarizes the statistical parameters calculated for all the cases. Agreement for the first two cases may be judged to be poor, however, the agreement for these cases suffers largely from significant under-prediction in the BATH zone. As expected, the agreement was consistently better for the cases with the HAC system operating. The individual zone average concentrations from all cases are also plotted in Figure 5 to summarize the comparison of predictions and measurements. The predicted SF_6 concentration averaged over all zones and cases (not weighted by zone volume) was within 10 % of the average measured concentration. Excluding the bathroom zone, the overall average predicted concentration 115 µg/m^3 (19.3 ppb(v)) was essentially identical to the overall average measured concentration 116 µg/m^3 (19.5 ppb(v)).

There are some important factors to consider before drawing conclusions as to CONTAMW's modeling capability from these tests. As discussed previously (Emmerich 2001), an absolute validation of a complex building airflow model, such as CONTAMW, is impossible because the user can create an infinite variety of models. However, one important reason to perform experimental validation is to identify and hopefully eliminate large errors. For the situations modeled in this effort, no large errors in the CONTAMW model were identified.

It is also important to remember that the ASTM D5157 guide is a guideline not an ultimate arbiter of model accuracy. Rather than the specific parameters and criteria, its primary value may be to move model validation beyond the all too common and oversimplified analysis of "the measurements and predictions differed by X %" and toward useful statistical analysis of model validation results.

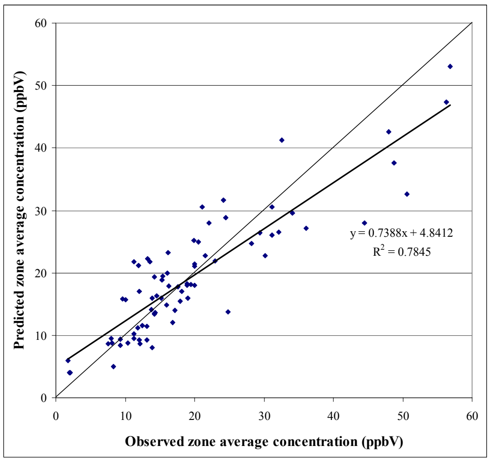

Figure 5 Comparison of Predicted and Measured zone average concentrations for all cases

Additionally, some of the discrepancies between model predictions and experimental measurements are due to experimental limitations instead of model deficiencies. For example, this effort involved a fairly rich data set in terms of number of variables monitored and spatial and temporal detail. Still, after completing the simulation effort, one can identify additional measurements that would have been desirable. Specifically, the halls and stairs of the townhouse provide the prime pathways for contaminant transport for cases without the HAC system operating – having temperature and concentration measurements in these important zones would have been valuable. Also, as previously discussed, inaccuracies in experimental measurements include much more than simply the instrument accuracy. All measurements reported here were a single point (often chosen to limit obtrusiveness to the occupants) that was used to represent an average room concentration. The ability of this single point measurement to represent the room is certainly questionable shortly after a major system perturbation (i.e., a quick injection of a large amount of tracer gas) or in the presence of continuous local disruption (i.e., location of a room sampling point in the path of ventilation supply air). Conduction of the experimental effort in an occupied home (although not occupied during the injection tests) presented the challenge of possessing less than complete control of the ‘laboratory’.

The model, while quite detailed, could have been more so. The simple air-handling system option of CONTAMW was used rather than the detailed duct model option. While it is unlikely this modeling choice affected the HAC system on cases, it may have affected the HAC system off cases as the idle ducts can act as an important airflow pathways between zones that otherwise have little or no direct communication. Additionally, some of the cases may have been affected by the CONTAMW 1.0 limitation of constant zone temperatures. While the interior temperature for most zones was stable during most tests, there were situations such as the second test case when the temperature difference between the 3rd floor and the attic ranged from 2°C – 5 °C during the test. It would be interesting to repeat simulations for selected cases with the newest version of CONTAMW 2.0, which includes the capability of varying zone temperatures according to a schedule.

Table 3 Summary of Statistical Parameters for All Cases

Case	HAC	C_o	C_p	σ_o	σ_p	R	m	b/C_o (%)	NMSE	FB	FS
1	Off	26.6	21.0	19	13	0.46	0.31	48	0.54	**-0.24**	-0.73
2	Off	32.2	25.0	12	8.4	0.81	0.57	**20**	**0.12**	**-0.25**	-0.67
3	Off	18.9	16.4	10	7.6	0.56	0.41	45	**0.24**	**-0.14**	**-0.52**
4	On	13.9	12.2	2.0	2.2	**0.88**	**0.96**	**-8.2**	**0.018**	**-0.13**	**0.19**
5	Off	17.7	16.6	5.7	7.2	0.75	**0.95**	**-1.5**	**0.07**	**-0.07**	**0.46**
6	On	17.9	16.7	2.5	3.2	**0.96**	**1.2**	**-32**	**0.01**	**-0.07**	0.51
7	On	13.5	14.5	2.1	3.1	**0.86**	**1.3**	**-21**	**0.02**	**0.06**	0.74
8	Off	14.5	12.1	14	12	**0.96**	**0.80**	**3.9**	**0.13**	**-0.17**	**-0.36**
9	Off	20.5	22.1	16	14	**0.91**	**0.78**	30	**0.10**	**0.11**	**-0.30**
10	On	20.9	26.5	6.9	10	**0.96**	1.4	**-16**	**0.08**	**0.23**	0.74

Finally, it is not necessary for this model evaluation to stand entirely on its own. Rather, it should be considered in the context of the existing body of work validating CONTAMW and similar models. Emmerich (2001) reviewed ten such efforts that have been reported in the literature. This validation effort differs from others reported primarily in number of variables monitored, number of cases analyzed, and execution of experimental effort in an occupied home. In the end, the results reported here echo those summarized in the earlier review: a knowledgeable user can expect to make reasonable predictions of air change rates, interzonal flows, and contaminant concentrations for residential-scale buildings dominated by stack-driven or ventilation flows with inert pollutants. Areas identified previously as needing more work such as large buildings, wind-driven flows, reactive contaminants, small time scales, and non-trace contaminants were not addressed in this study. Some of these needs are being addressed by ongoing research at NIST.

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